Progress towards a new international standard for storing nuclear data

CSEWG 2016

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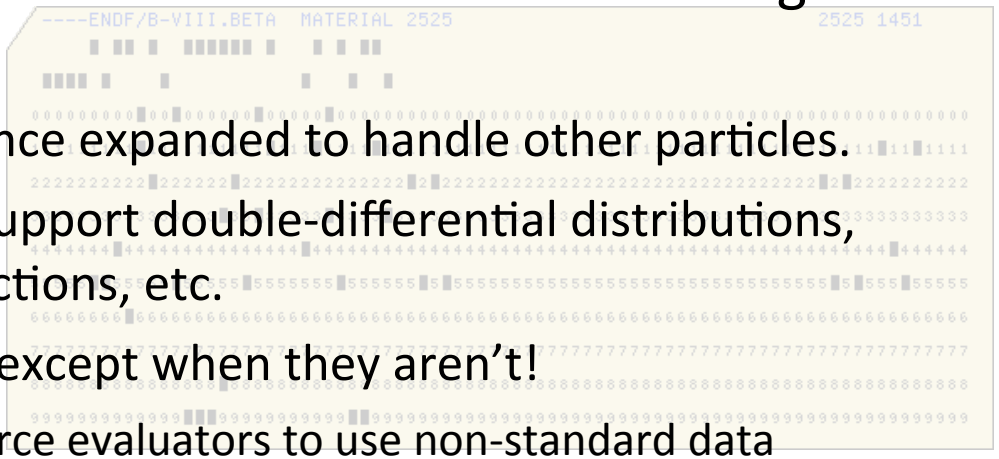
Motivation: the ENDF-6 format is having trouble keeping up with expanding needs of nuclear data users.

- For over 50 years, ENDF-6 has been the standard for storing and exchanging nuclear data
  - Originally neutrons only, has since expanded to handle other particles.
  - Format gradually modified to support double-differential distributions, covariances, more types of reactions, etc.
  - Data are computer-readable... except when they aren't!
    - Format limitations sometimes force evaluators to use non-standard data representations like the 'LIP' product modifier flag: "The exact meaning assigned to LIP should be explained in the File 1, MT=451 comments"
  - Despite format checking codes, bugs in ENDF-6 evaluations remain difficult to find and fix!



- New generation of nuclear data experts asks for modern tools to handle data!

Original proposal to WPEC by McNabb:

LLNL has made an initial attempt at a new format, which can be downloaded at https://ndclx4.bnl.gov/gf/project/gnd/

- Sub-group participants will
  - Develop a common data model for reaction data
  - Agree on best practices and how to “enforce” them
  - Test things out with their local ENDF-formatted databases
  - Propose a process for dissemination and future modifications
- LLNL and USNDP is committed to seeing this through
- Benefits are significant
  - Attract and retain next generation of scientists and engineers
  - Leverage significant infrastructure that will continue to evolve
  - Overcomes limitations of existing format in an extensible way
  - Positions community to link disparate data products to each other

WPEC subgroup #38 was approved in May 2012, and has since met seven times (plus multiple phone conferences)

- Meetings mainly held at the NEA (Paris), but also at JAEA, BNL, IAEA and OECD
- Contributors from all data projects joined in the discussions.

SG38 work was divided into several sub-tasks:

- Low-level data containers
  - Similar to ENDF LIST, TAB1, TAB2, etc.
  - Work with other data projects (e.g., ENSDF, EXFOR, RIPL)
- Hierarchy for storing particle data and nuclear level schemes and decay data
- Top-level hierarchy for storing nuclear reaction data
- Infrastructure for data handling, processing, plotting, etc.
- API for reading and writing data in the new structure
- Defining the tests that will be needed to assure quality of data
- Documentation and governance

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Nearly complete

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Continued in SG43

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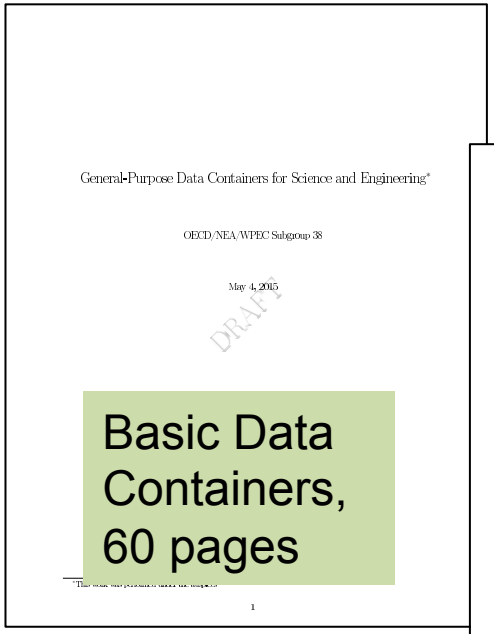
SG-B is being revived to provide long-term governance

SG38 will be completed with the publication of 4 ‘requirements and specifications’ documents

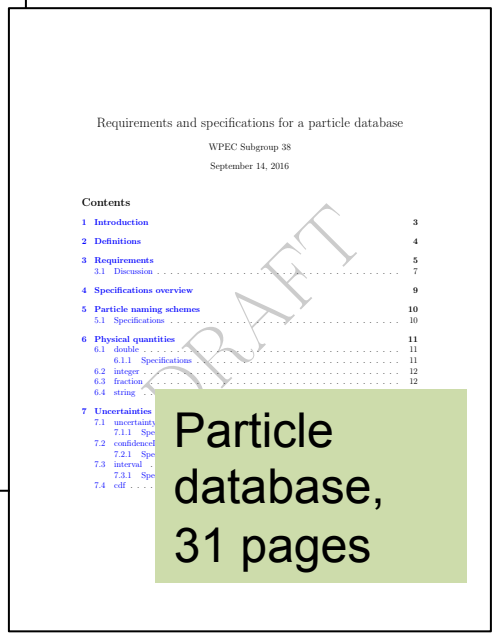

General-Purpose Data Containers for Science and Engineering*

OECD/NEA/WPEC Subgroup 38

May 4, 2015

DRAFT

Basic Data Containers, 60 pages


Requirements and specifications for a particle database

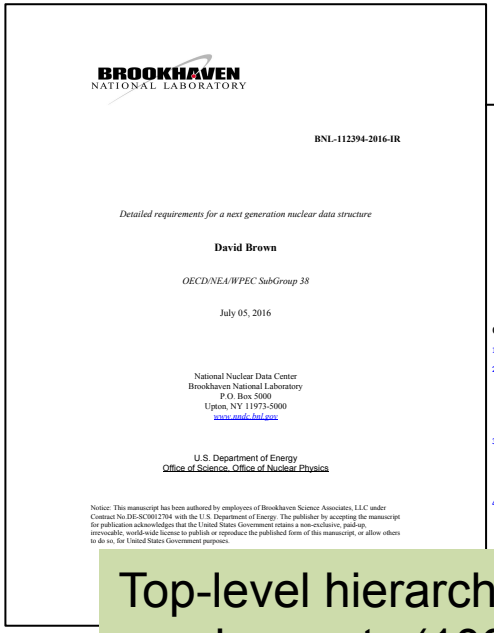
WPEC Subgroup 38

September 14, 2016

Contents

DRAFT

Particle database, 31 pages


BROOKHAVEN NATIONAL LABORATORY

BNL-112394-2016-IR

Detailed requirements for a next generation nuclear data structure

David Brown

OECD/NEA/WPEC SubGroup 38

July 05, 2016

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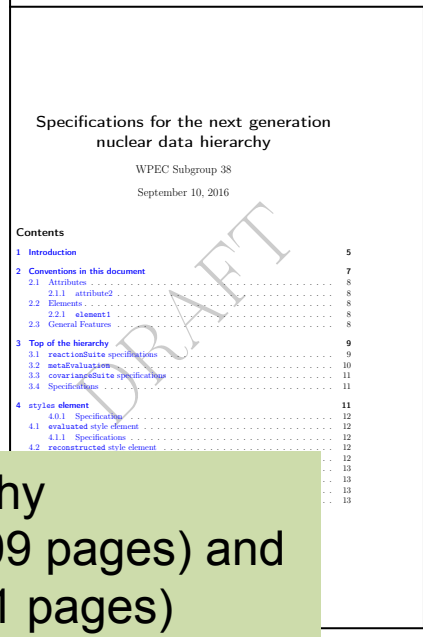
U.S. Department of Energy
Office of Science, Office of Nuclear Physics


Specifications for the next generation nuclear data hierarchy

WPEC Subgroup 38

September 10, 2016

Contents

DRAFT

Top-level hierarchy requirements (109 pages) and specifications (61 pages)

- All available at https://www.oecd-nea.org/science/wpec/sg38/

Brief overview of some SG38 specifications: basic data containers

- 1-d functions (such as cross section and nubar) are stored as a list of (x,y) pairs with interpolation:

```
<XYs1d label="eval" style="eval" interpolation="lin-lin">
 − <axes>
      <axis label="energy_in" unit="eV"/>
      <axis label="crossSection" unit="b"/>
   </axes>
 − <values length="164">
      128262 0 1.3e5 0.0615264 1.4e5 0.225903 1.5e5 0.322846 2e5 0.561636 ... 5.5e7 7.56553e-3 6e7 6.81747e-3
   </values>
 + <uncertainties></uncertainties>
</XYs1d>
```

- Changing interpolations are handled with a ‘regions’ container:

```
<regions1d label="eval" style="eval">
 − <axes>
      <axis label="energy_in" unit="eV"/>
      <axis label="crossSection" unit="b"/>
   </axes>
 + <XYs1d interpolation="log-log"></XYs1d>
 + <XYs1d interpolation="lin-lin"></XYs1d>
 + <uncertainties></uncertainties>
</regions1d>
```

Brief overview of some SG38 specifications: basic data containers

- 2-d functions (i.e. outgoing energy distributions) are similar to TAB2, composed of 1-d functions along with an interpolation rule:

```
<XYs2d interpolation="lin-lin" interpolationQualifier="unitbase">
 − <axes>
      <axis label="energy_in" unit="eV"/>
      <axis label="energy_out" unit="eV"/>
      <axis label="P(energy_outlenergy_in)" unit="1/eV"/>
   </axes>
 + <XYs1d value="2969996.0" interpolation="lin-lin"></XYs1d>
 + <XYs1d value="3000000.0" interpolation="lin-lin"></XYs1d>
   ...
 + <XYs1d value="55000000.0" interpolation="lin-lin"></XYs1d>
 + <XYs1d value="60000000.0" interpolation="lin-lin"></XYs1d>
</XYs2d>
```

- Other data containers include series (i.e. Legendre expansions and other polynomials), multi-dimensional arrays, 'gridded' arrays (used to store covariances and transfer matrices), and tables (for resonance parameters)

Brief overview of SG38 specifications: overall organization of data

- GND ‘reactionSuite’ is similar to ENDF-6 ‘MAT’. Data inside the reactionSuite are organized in a nested hierarchy

```
– <reactionSuite projectile="n" target="Mn55" version="GND 1.7" projectileFrame="lab">
  + <styles></styles>
  + <documentations></documentations>
  + <aliases></aliases>
  + <particles></particles>
  + <resonances reconstructCrossSection="true"></resonances>
  + <reactions></reactions>
  + <sums></sums>
  + <productions></productions>
  </reactionSuite>
```

Brief overview of SG38 specifications: overall organization of data

- Largest section is <reactions>, containing the list of all reactions that sum to total:

```
<reactions>
 + <reaction label="0" outputChannel="n + Mn55" date="2011-02-01" ENDF_MT="2"></reaction>
 + <reaction label="1" outputChannel="n + Mn55_e1" date="2011-02-01" ENDF_MT="51"></reaction>
 + <reaction label="2" outputChannel="n + Mn55_e2" date="2011-02-01" ENDF_MT="52"></reaction>
 + <reaction label="3" outputChannel="n + Mn55_e3" date="2011-02-01" ENDF_MT="53"></reaction>
 + <reaction label="4" outputChannel="n + Mn55_e4" date="2011-02-01" ENDF_MT="54"></reaction>
 + <reaction label="5" outputChannel="n + Mn55_e5" date="2011-02-01" ENDF_MT="55"></reaction>
 + <reaction label="6" outputChannel="n + Mn55_e6" date="2011-02-01" ENDF_MT="56"></reaction>
 + <reaction label="7" outputChannel="n + Mn55_e7" date="2011-02-01" ENDF_MT="57"></reaction>
 + <reaction label="8" outputChannel="n + Mn55_e8" date="2011-02-01" ENDF_MT="58"></reaction>
 + <reaction label="9" outputChannel="n + Mn55_e9" date="2011-02-01" ENDF_MT="59"></reaction>
   ...
```

Brief overview of SG38 specifications: contents of a 'reaction'

- Each reaction stores a cross section and an outputChannel (with a Q-value and a list of products):

```
<reactions>
 − <reaction label="0" outputChannel="n + Mn55" date="2011-02-01" ENDF_MT="2">
   + <crossSection></crossSection>
   − <outputChannel genre="twoBody">
     + <Q></Q>
     − <products>
       − <product name="n" label="n">
         + <multiplicity></multiplicity>
         + <distribution></distribution>
         </product>
       − <product name="Mn55" label="Mn55" ENDFconversionFlag="implicitProduct">
         + <multiplicity></multiplicity>
         + <distribution></distribution>
         </product>
       </products>
     </outputChannel>
   </reaction>
 + <reaction label="1" outputChannel="n + Mn55_e1" date="2011-02-01" ENDF_MT="51"></reaction>
   …
```

Brief overview of SG38 specifications: using 'styles' to store more than one type of data

- GND can store various types of processed data along with evaluated data. 'styles' section has a directory of data types:

```
<styles>
 + <evaluated label="eval" date="2011-02-01" library="ENDF/B" version="8.0.2"></evaluated>
   <crossSectionReconstructed label="recon" derivedFrom="eval" date="2016-09-14"/>
 - <heated label="h1" derivedFrom="eval" date="2016-09-14">
     <temperature value="3.e2" unit="K"/>
   </heated>
 - <heated label="h2" derivedFrom="eval" date="2016-09-14">
     <temperature value="1.2e3" unit="K"/>
   </heated>
</styles>
```

- Each data style may appear inside crossSection, multiplicity, distribution, etc.

```
<crossSection>
 + <resonancesWithBackground label="eval" style="eval"></resonancesWithBackground>
 + <XYs1d label="recon" style="recon"></XYs1d>
 + <XYs1d label="h1" style="h1" accuracy="0.002"></XYs1d>
 + <XYs1d label="h2" style="h2" accuracy="0.002"></XYs1d>
</crossSection>
```

SG38 work will continue with new subgroup #43 and long-term subgroup B:

- Low-level data containers
  - Similar to ENDF LIST, TAB1, TAB2, etc.
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SG-B is being revived to provide long-term governance

New subgroups will officially start in May 2017. Now working to define their goals and scope:

- SG-B
  - From proposal: "… propose that a new WPEC long-term subgroup become the stewards of a new international standard for a modern nuclear database structure."
    - Endorse, promote and maintain the new format. Includes facilitating training and education for evaluators, and approving and adopting future changes.

- SG43
  - Provides infrastructure to accompany the new format. Main goals:
    - Design and implement an API to read and write GND-formatted files
    - Define a list of tests (including data format tests and physics tests) that need to be implemented for data quality assurance.

SG-38 produced a format specification, now focus turns to disseminating the format and building infrastructure.

- SG-38 requirements and specifications documents under final revision, will be published soon
- SG-B takes on format governance
- SG-43 expands the infrastructure for generating, checking, manipulating and using GND-formatted data


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